UCRL-CONF-214079

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The Piecewise Linear Reactive Flow Rate Model

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July 28, 2005

14th APS Conference on Shock Compression of Condensed Material
Baltimore, MD, United States
July 31, 2005 through August 5, 2005

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This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

Motivation for new reactive flow rate models for non-ideal explosives

- A wide range of behavior is observed in non-ideal explosives experiments dealing with differing sizes and geometries.
- These experiments sample different regions of the phase space in the detonation wave.
- A good predictive detonation model should be able to reproduce the many observed phenomena including
  - variations in the detonation velocity with the radial diameter of rate-sticks.
  - slowing of the detonation velocity around gentle corners.
  - production of dead zones for abrupt corner turning.
  - failure of small diameter rate sticks.
  - crack detonation transmission and damping.
  - initiation.

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Goal for a true predictive model

- Currently most detonation modeling is done using
  - program burn models with phenomenological equations of state.
  - simple reactive flow models.
- These models have been developed to explain one effect at a time.
- Often, changes are made in the input parameters used to fit each succeeding case, with the implication that this is sufficient for the model to be valid over differing regimes.
- For true predictive capabilities we feel that it is important to develop models that are able to fit all experiments with one set of parameters.

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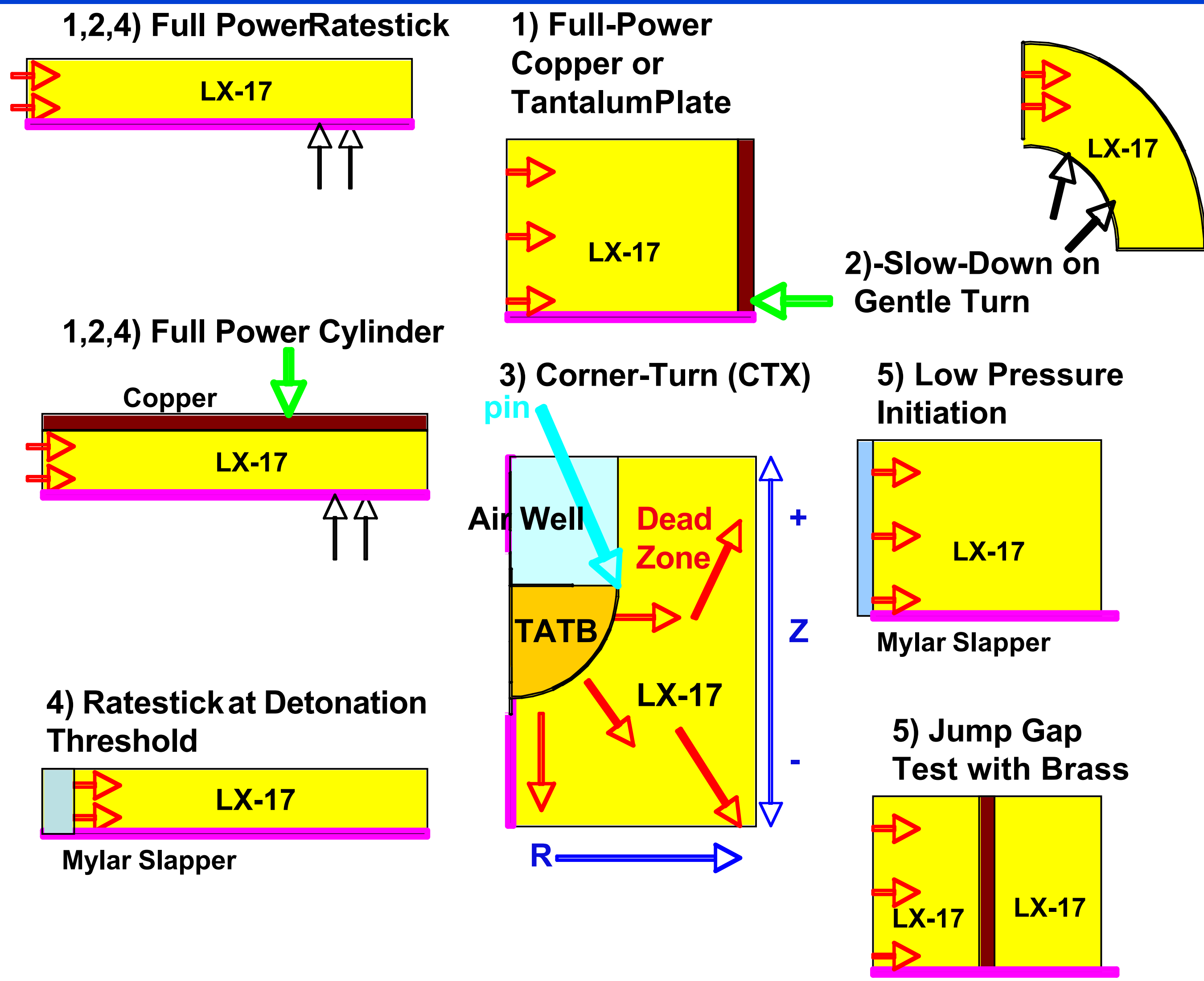
Small scale experiments provide a broad range of conditions for validation



The JWL++ rate model is adequate for strong detonation waves and simple geometries

- Our JWL++ model was developed as simple reactive flow rate model that could handle prompt detonation (i.e. strong detonation waves)
- This model treats the transition from an un-reacted Murnahan EOS to a JWL EOS using a single pressure power-law form rate law

$$\frac{dF}{dt} = AP^{B}(1-F)^{C}$$

- The variables A, B, and C are explosive dependent constants.
- *Because of the highly non-linear behavior of detonation waves of different strengths, one set of A, B, C constants does not fit a broad range of experimental conditions.*

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The Piece Wise Linear Reactive Flow Model (JWL++PWL) was developed to expand the range of applicability of the JWL++ model

- As with the JWL++ model we desired to keep the Piece Wise Linear reactive flow model as simple as possible.
- What was done was a generalization of the pressure power law term to a piece-wise linear function and the addition of a low pressure de-sensitization rate.
- The rate law connecting the un-reacted to reacted EOS is now:

$$\frac{dF}{dt} = AG(P)(1-F)^C$$

$$G(P) = \sum_{i=1..N} \Gamma_i$$

$$\Gamma_i = G_{i+1}\frac{(x - x_i)}{(x_{i+1} - x_i)} + G_i\frac{(x_{i+1} - x)}{(x_{i+1} - x_i)}$$

- The coefficients G_i are determined by calibration with experiments.

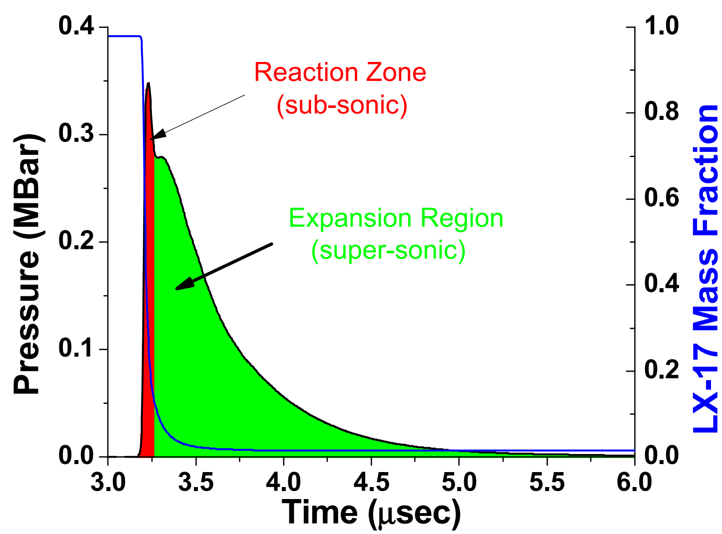
The Piece Wise Linear (PWL) Model includes low pressure de-sensitization.

- At low pressure, shock wave tend to de-sensitize inhomogeneous explosives by destroying hot spot ignition sites.
- To account for this affect in the PWL model
  - we set the normal burn rate dF/dt equal to zero below a cut-off pressure
  - apply a de-sensitization rate below the cut-off that transforms the un-reacted explosive to an inert form that does not burn.
- The PWL therefore follows three species
  - normal un-reacted.
  - inert un-reacted.
  - fully reacted.
- The de-sensitization rate is essential in explaining dead zone behavior in sharp corner turning experiments.

Calibrating the Piece Wise Linear Model requires data for different detonation wave strengths.

- Non-ideal detonation wave consists of a narrow reaction zone followed by super-sonic expansion regime
- The detonation wave behavior is sensitive to conditions only within the reaction zone
- Small scale experiments provide a broad range of conditions for validation which sample different reaction zone pressures
- For the PWL model we have used ignition data, rate-stick experiments, and the CTX corner turning data to initially calibrate the pressure rate coefficients.

On axis pressure and un-reacted mass fraction histories from a LX-17 rate-stick simulation



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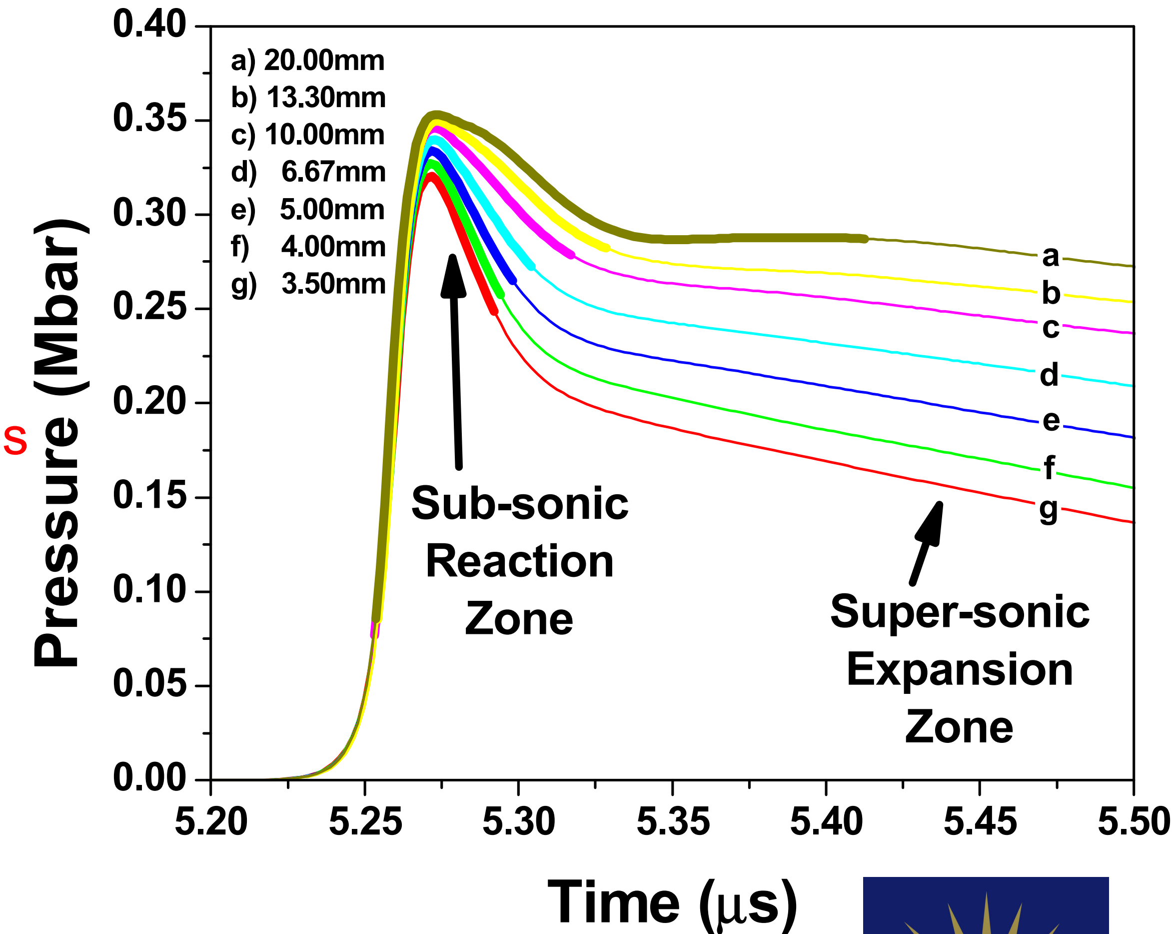
Reaction zone pressure regime shifts with detonation wave strength (LX-17 on axis JWL++PWL Model)

Rate-stick modeling shows that the pressure range in the reaction zone decreases with the strength of the detonation wave.

The wave strength decreases with decreasing rate-stick radius.

Rate-sticks can therefore be used to sample a pressure dependent rate model for strong (large rate-stick) to moderately weak waves (rate-stick near failure).



Rate-sticks provide a simple geometry for calibrating reactive flow rate models for strong to moderately weak detonation waves

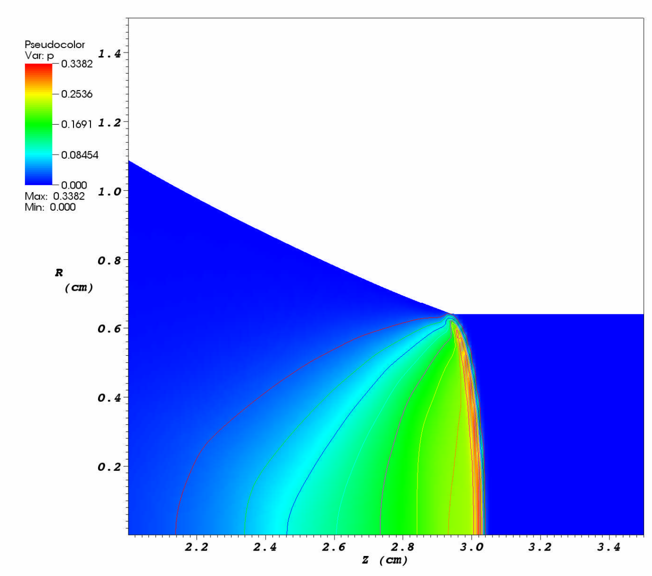
A typical pressure profile for a rate-stick shows a narrow high pressure reactive zone with slow radial variation of peak pressure.

A given rate-stick provides a means to probe a pressure dependent rate model over a small range of pressures

Starting with near-failure diameter small rate-sticks, and moving to large diameters shifts this probing to increasing pressures.

Values of the rate pressure coefficients can be calibrated at increasingly larger pressures by this technique

LX-17 rate-stick simulation



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Calibrating the mass fraction factor

- The mass fraction factor, $(1\text{-}F)^C$, in the PWL rate law specifies the how rapidly the burn rate goes to zero as the mass fraction of un-reacted material is depleted.

- In actual usage, $(1\text{-}F)^C$ is replaced by F_U^C, where F_U is the un-reacted mass fraction.

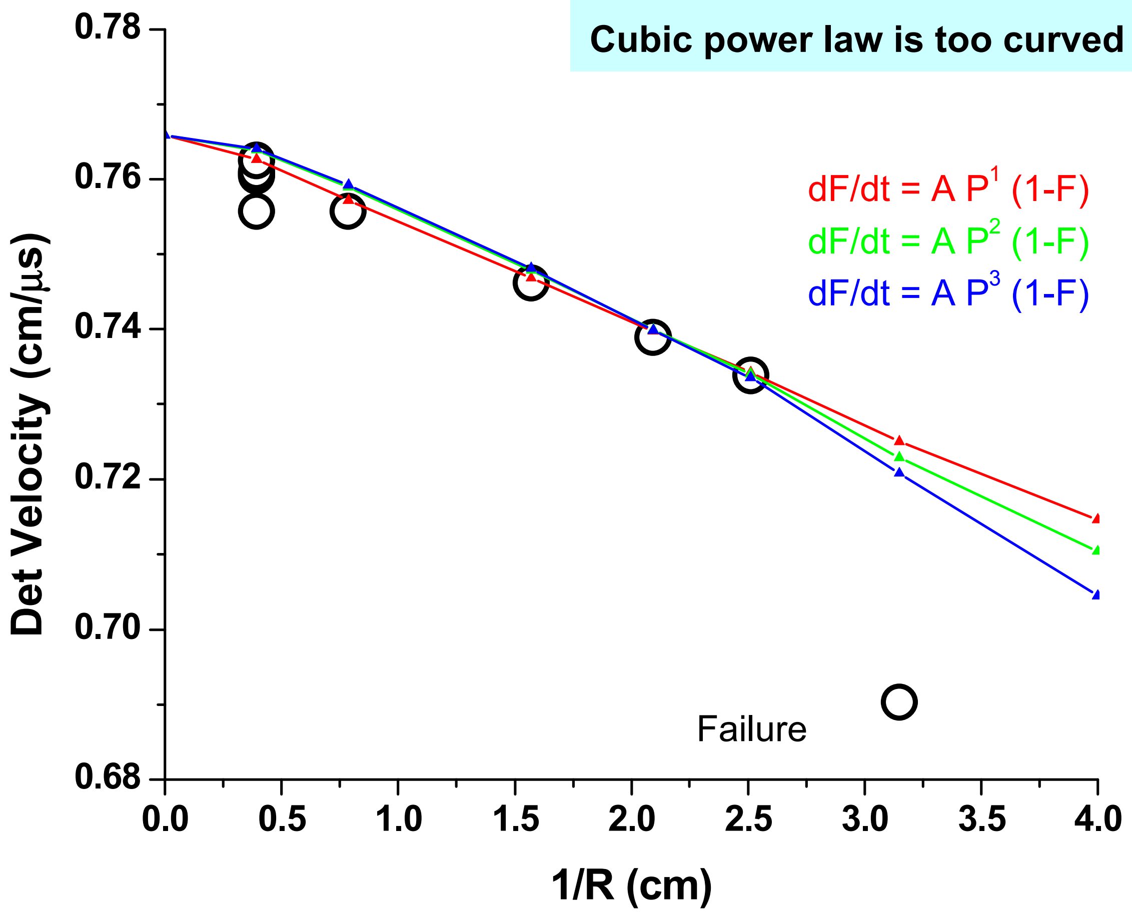
- Typical values in the past for C are < 1. We find that such values lead to excessive downward curvature when fitting rate-sticks for LX-17.

- Use of C > 1
  - reduces this curvature.
  - simulates a very slow, long time energy release which is believed to be caused by solid phase kinetics in carbon rich explosives

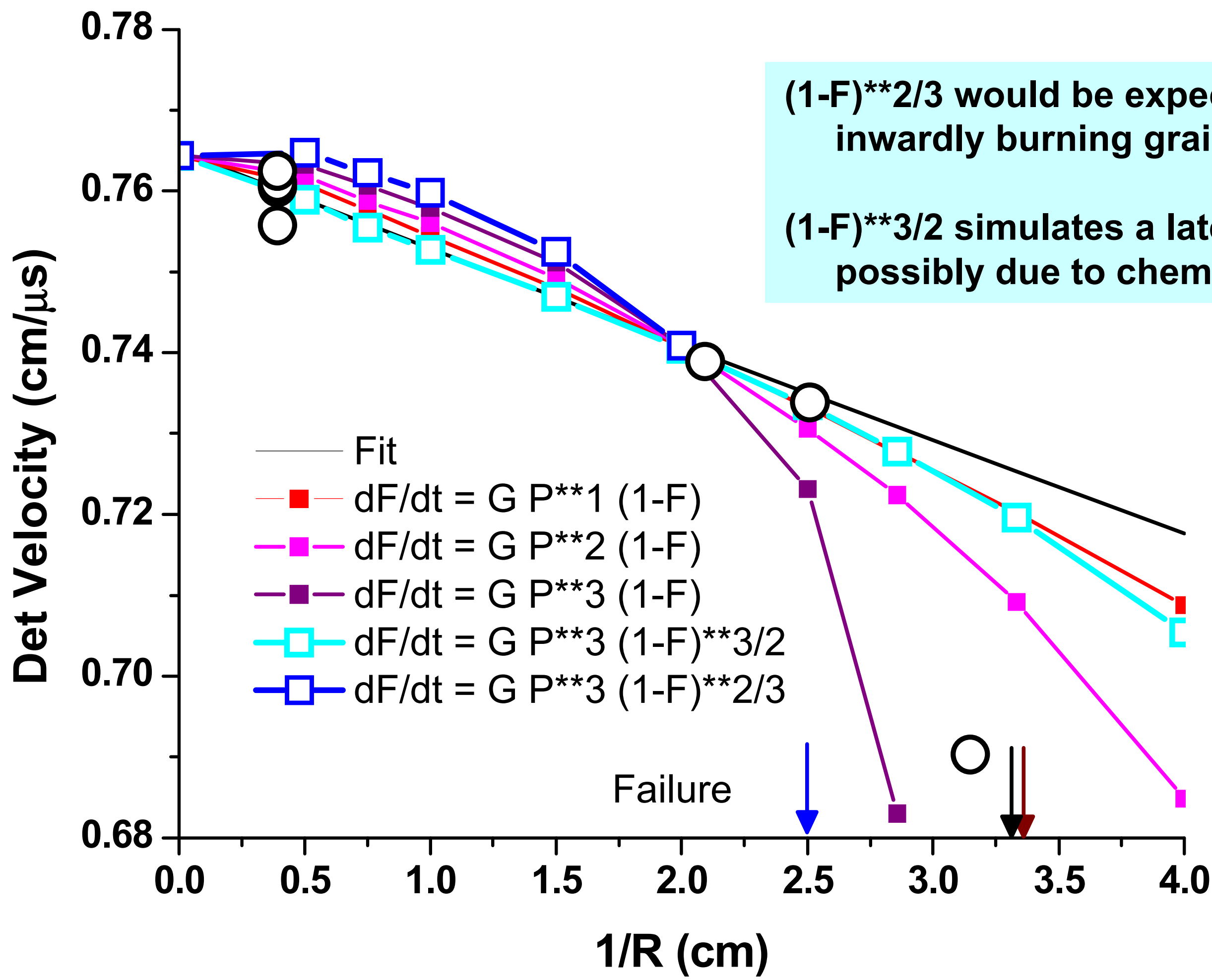
Pressure power law rates show too much curvature (Confined LX17 Rate Stick Fitting Using JWL++)

Linear power law has a nice flat fall off, but does not fail.

Cubic power law is too curved and fails too gradually.



Burn fraction form factor power law has the opposite behavior of the pressure power law

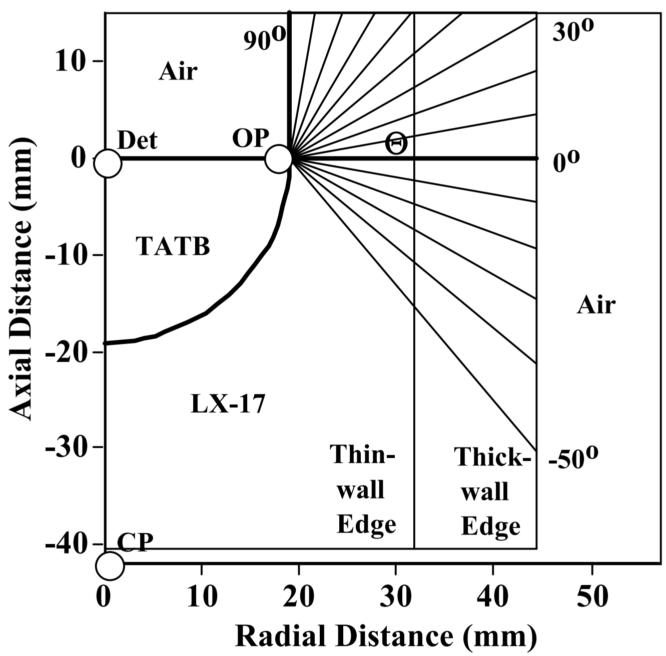


(1-F)**2/3 would be expected for inwardly burning grains

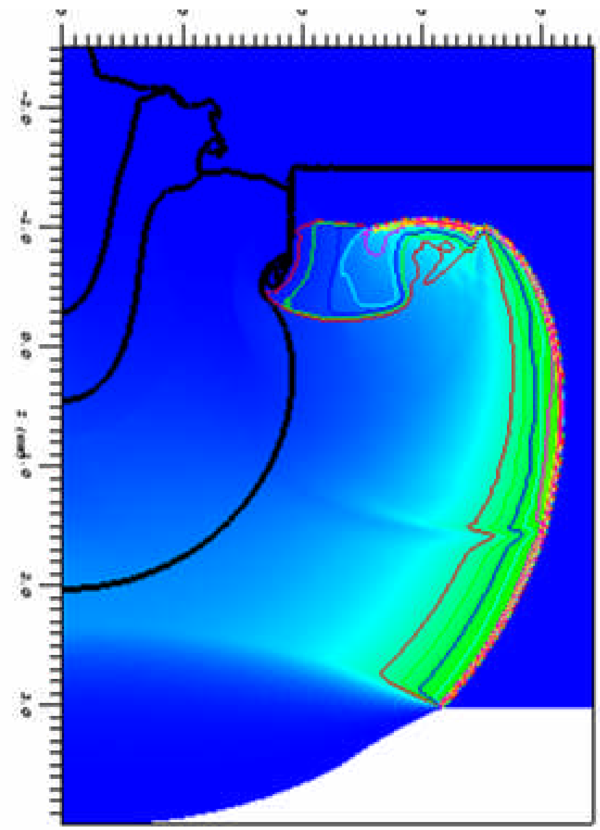
(1-F)**3/2 simulates a late time slowing possibly due to chemistry

CTX experiment supplies x-ray density radiograph and wall break-out timing data

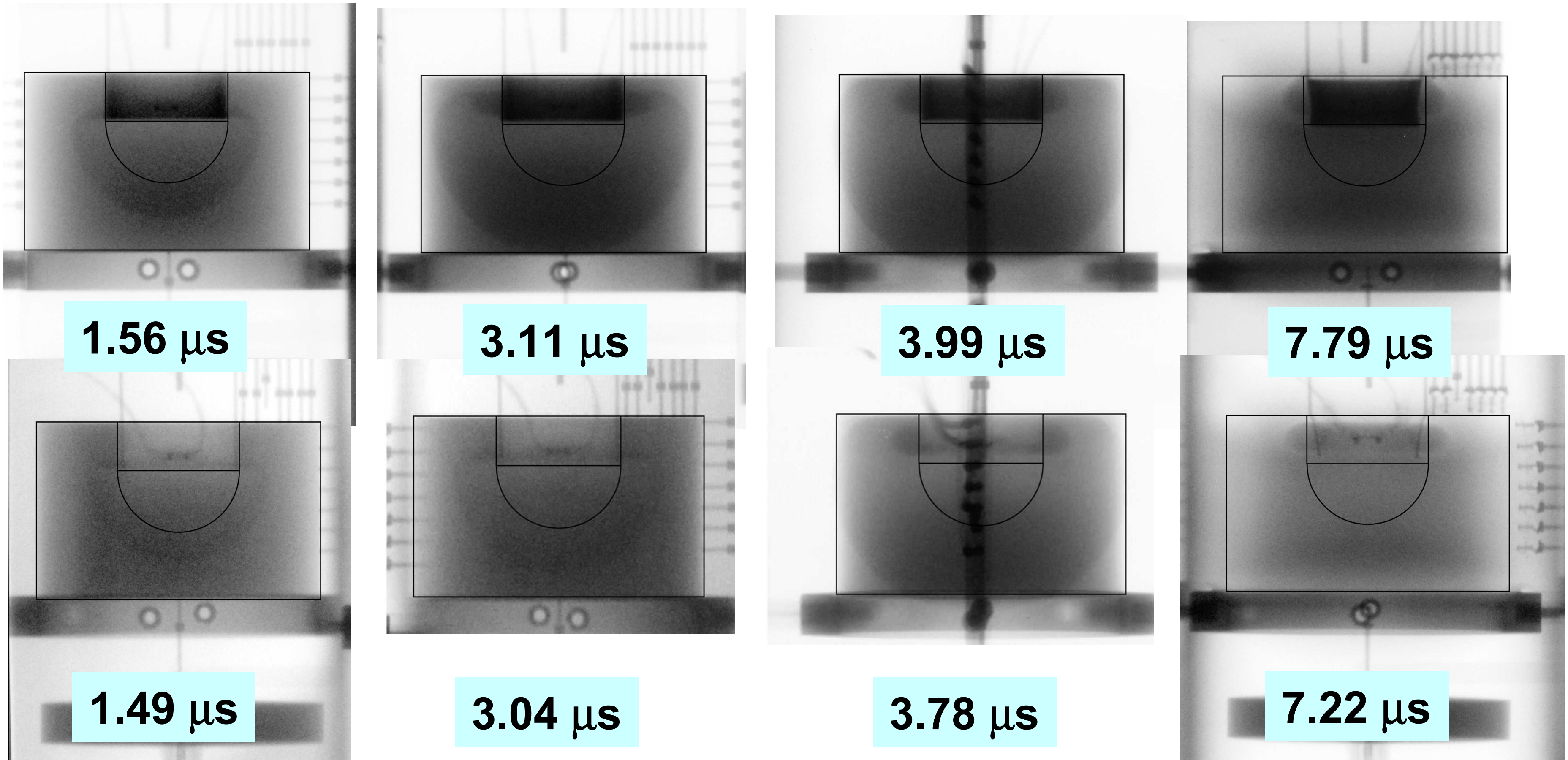
Experiment Geometry



Simulation pressure and density profiles



CTX experiment data for LX-17 cylinder with and without steel



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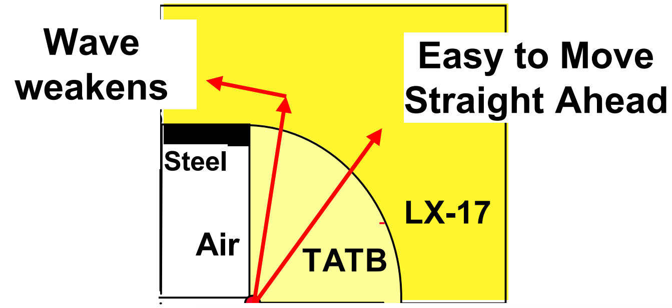
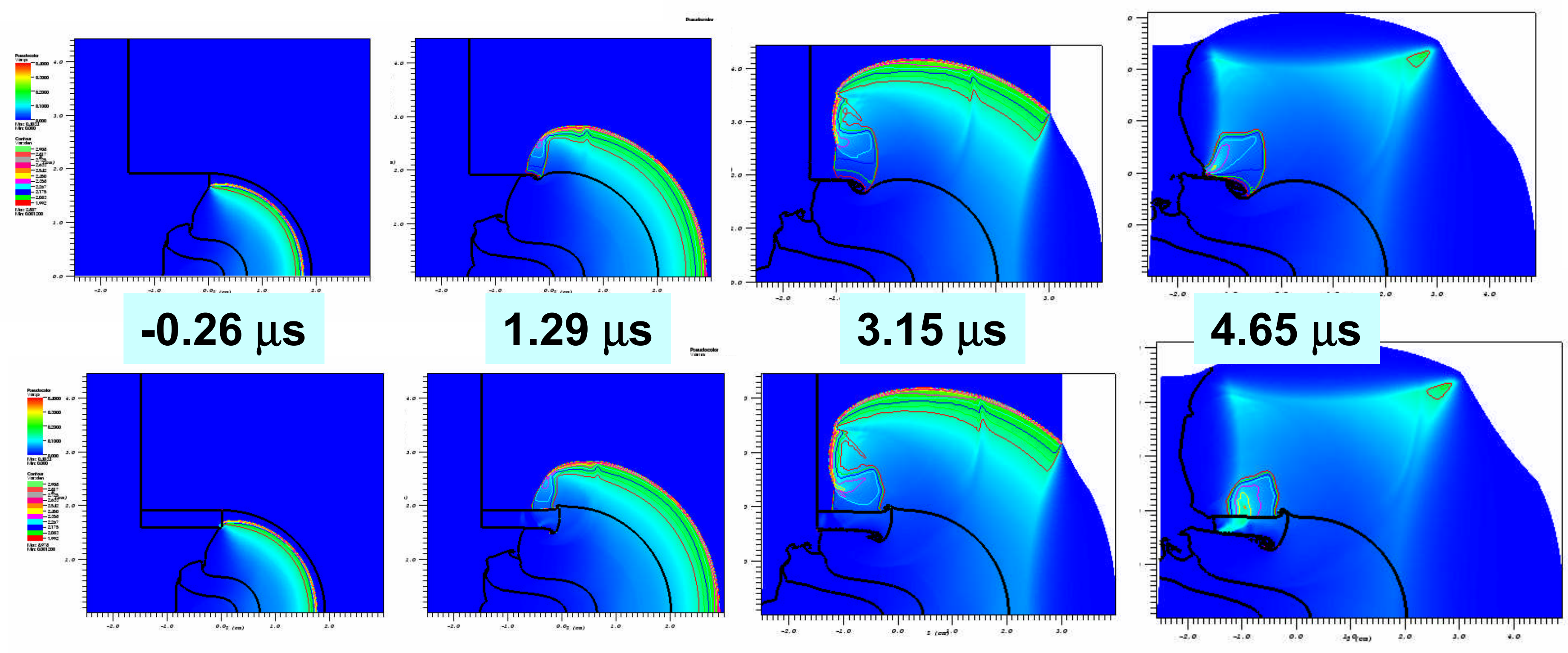
CTX simulation data for LX-17 cylinder with (lower) and without (upper) steel showing the formation of the dead zone

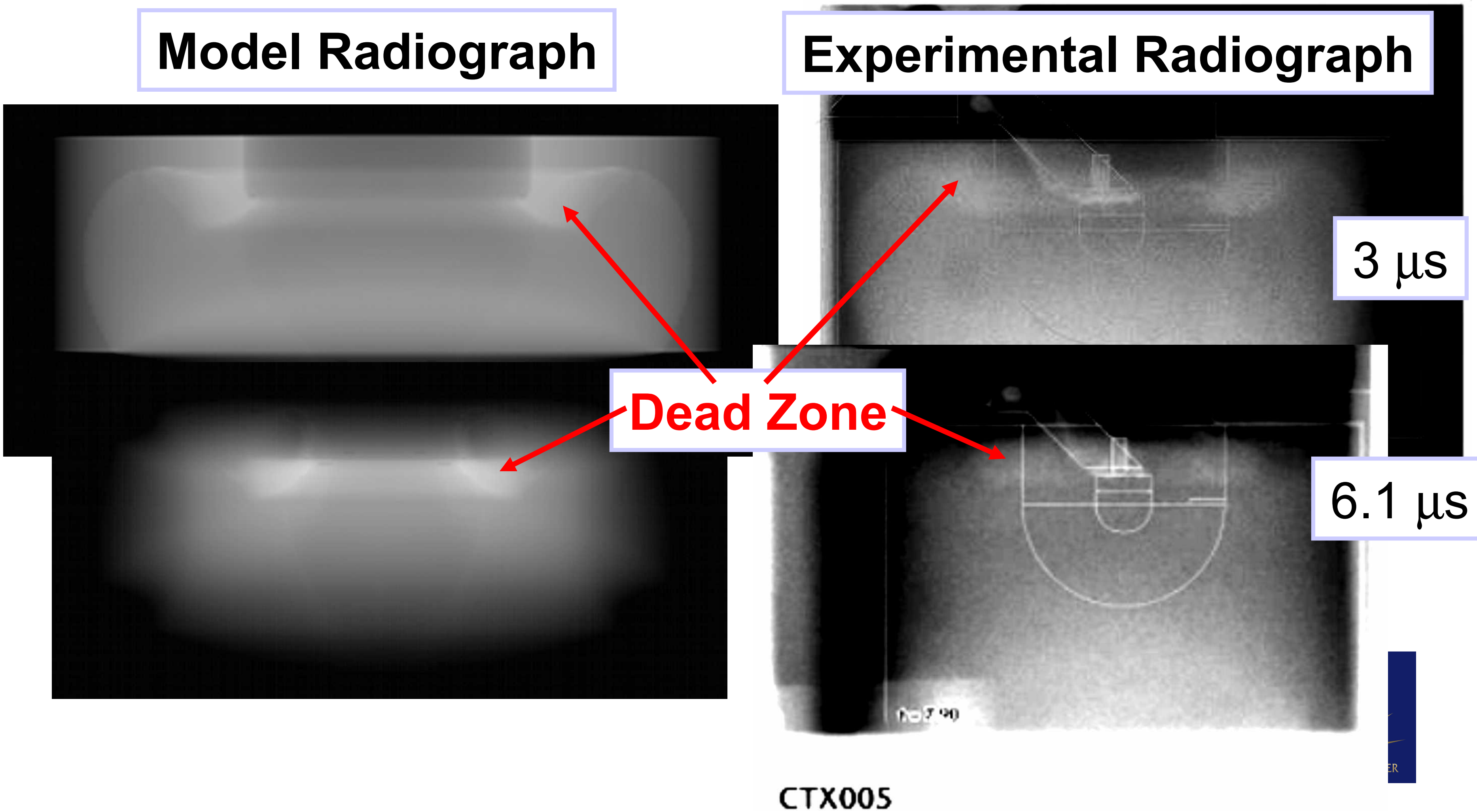
CTX hockey puck experiment uses hemisphere of TATB to ignite LX17.

Explores corner turning behavior.

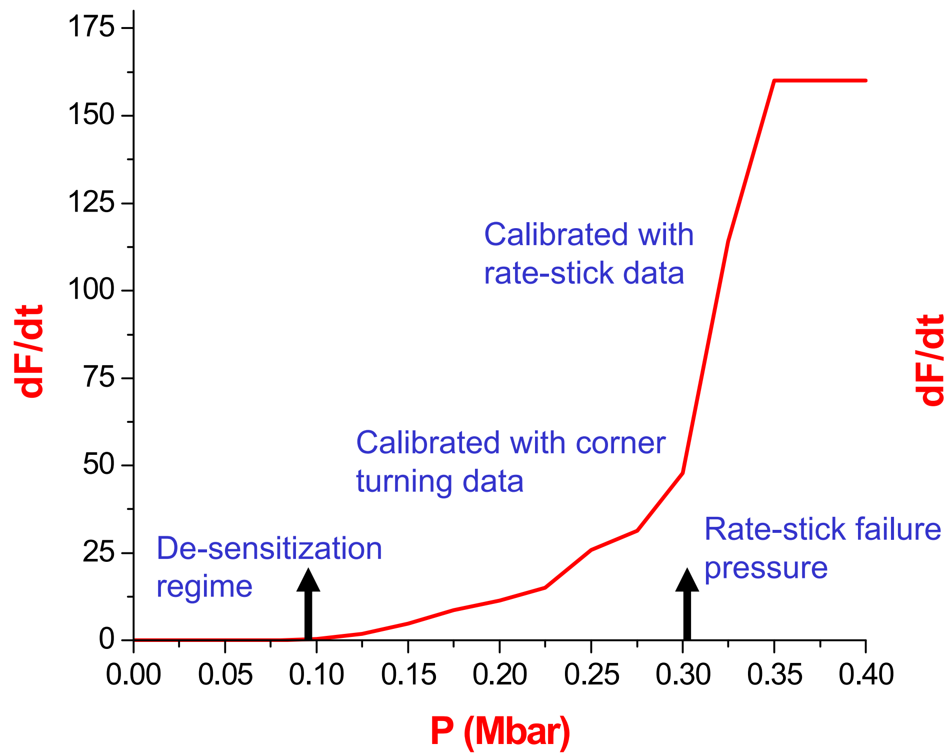


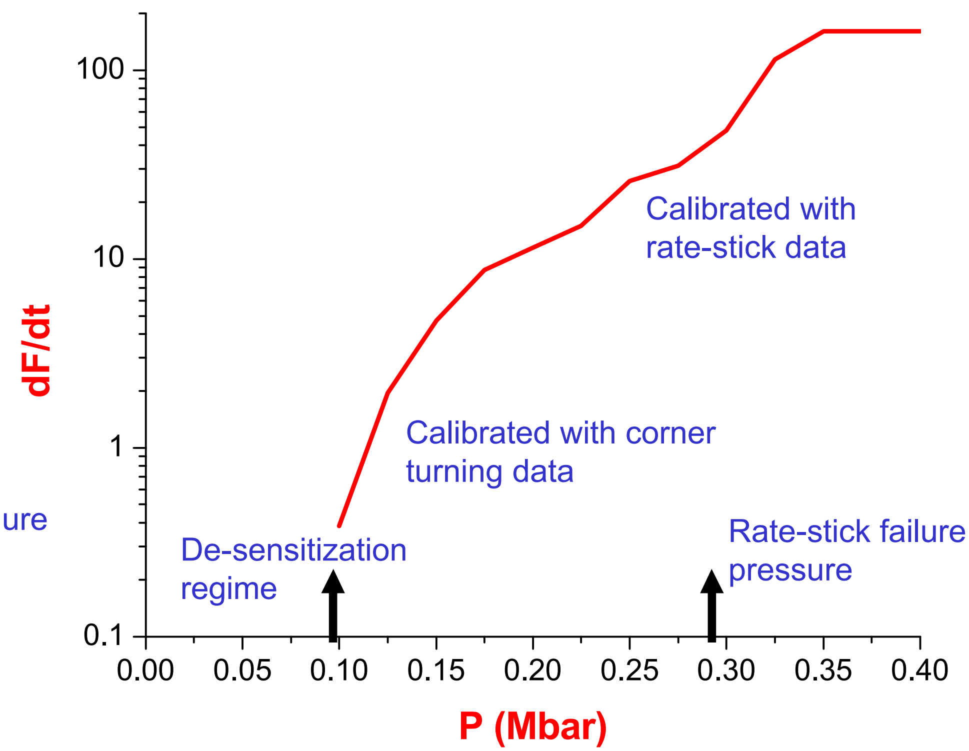


LX-17 hockey puck radiograph comparisons showing the dead zone

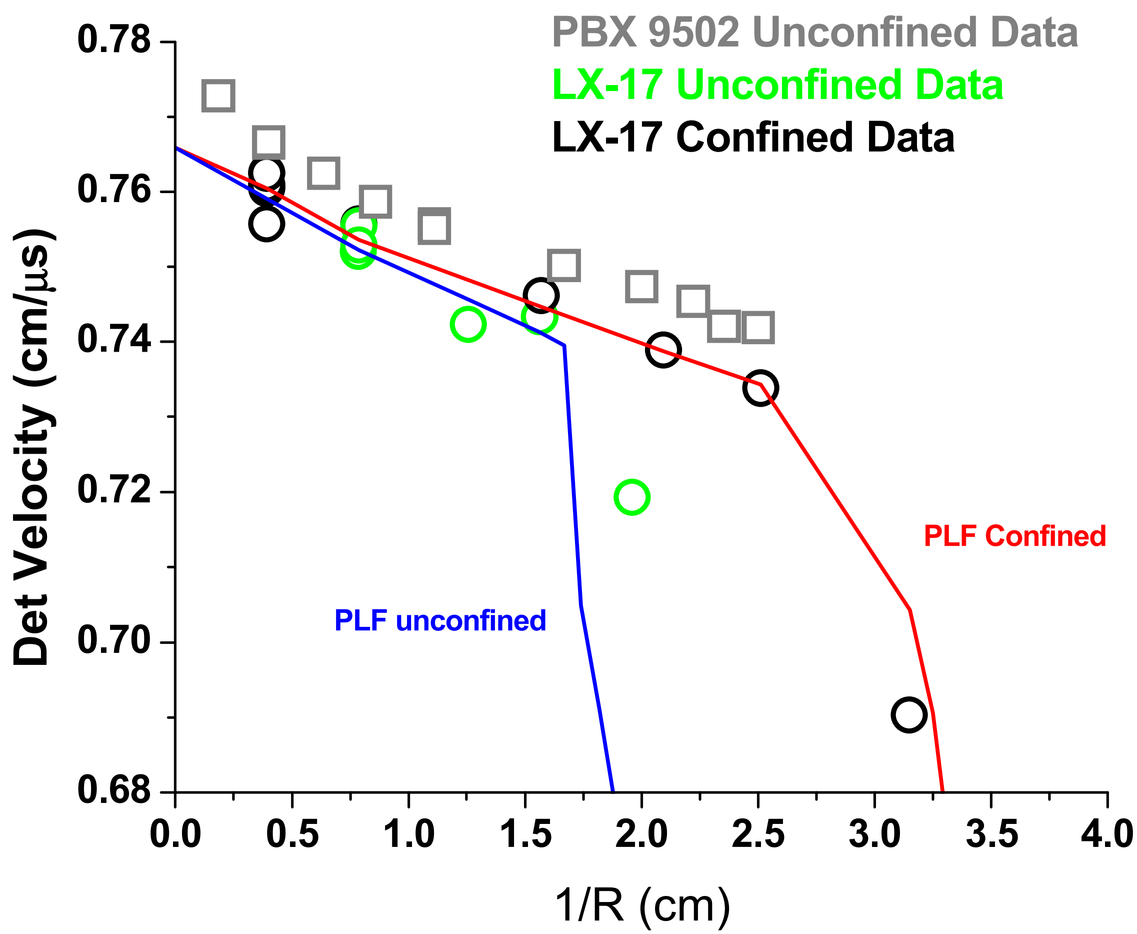


Piece Wise Linear pressure rate for LX-17





PWL size effect modeling for LX-17 rate-sticks Gives excellent agreement including abrupt failure



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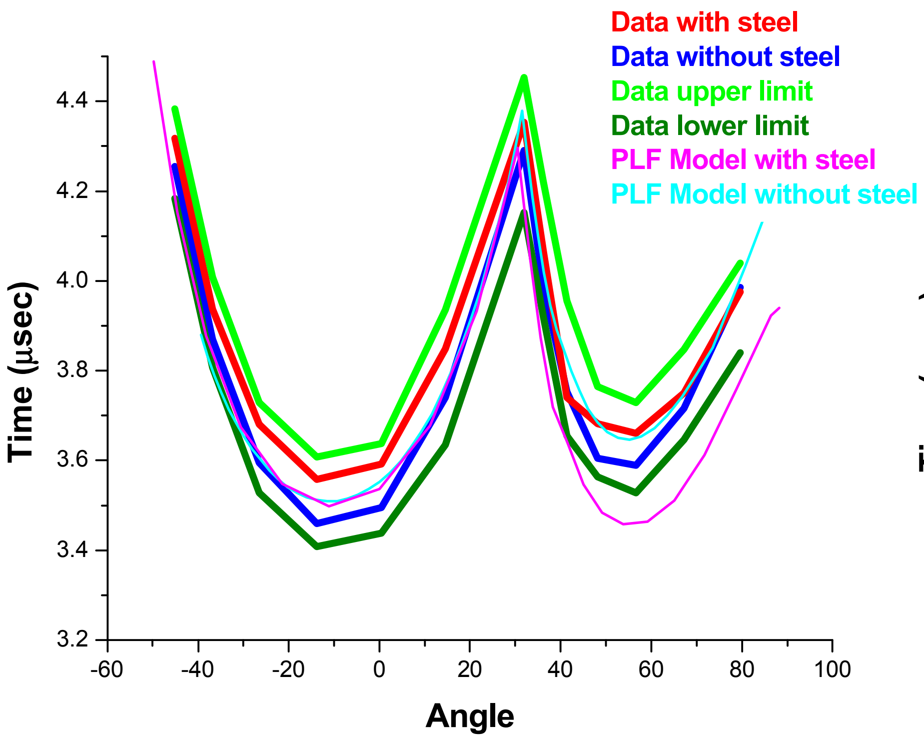
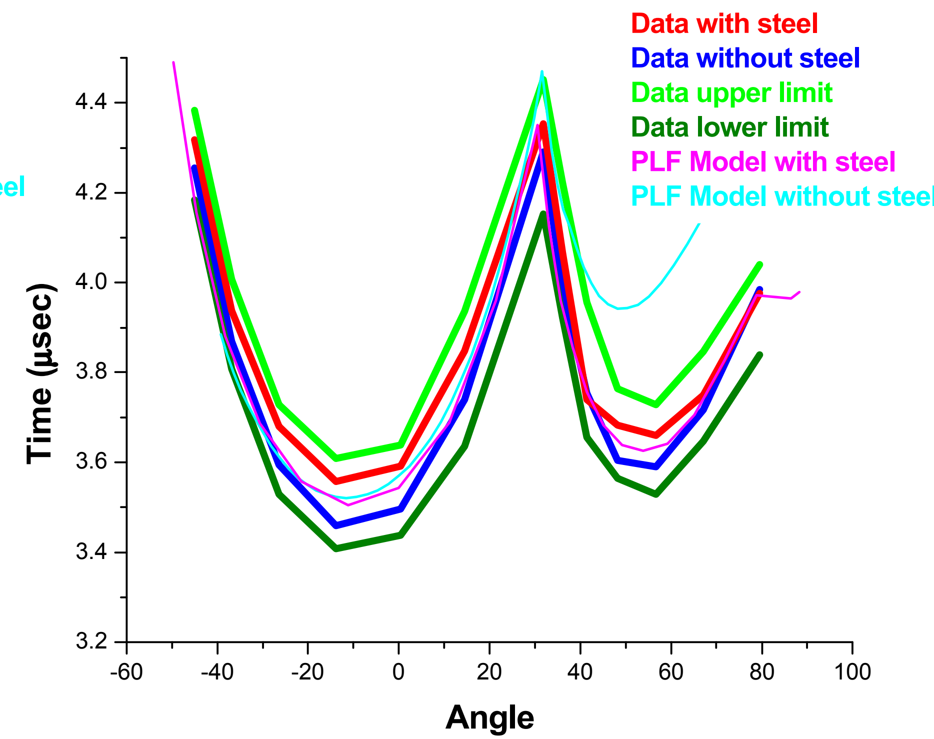
Corner Turning Modeling for the Hockey Puck Booster Experiment (LX-17)





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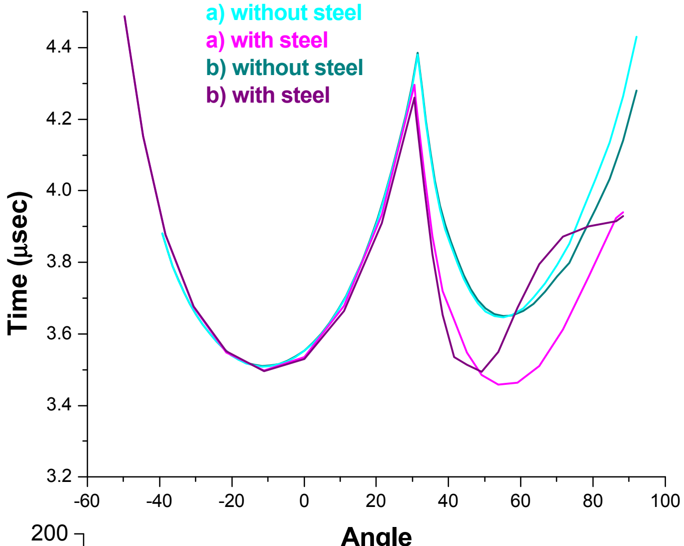
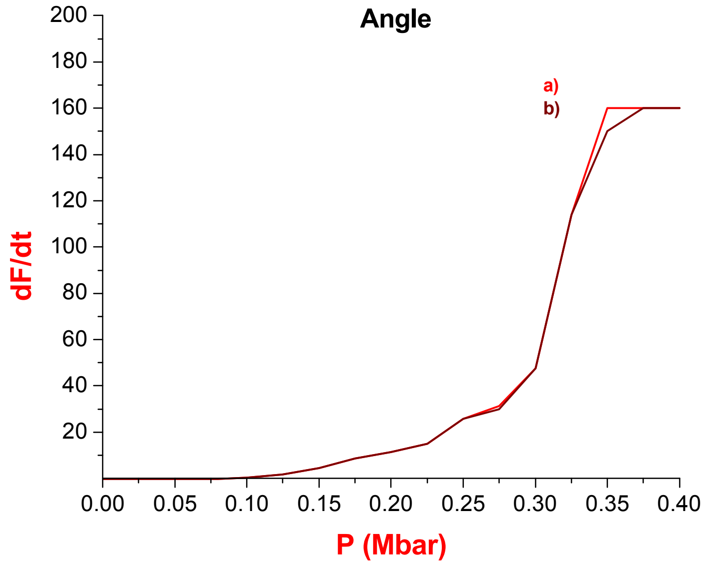
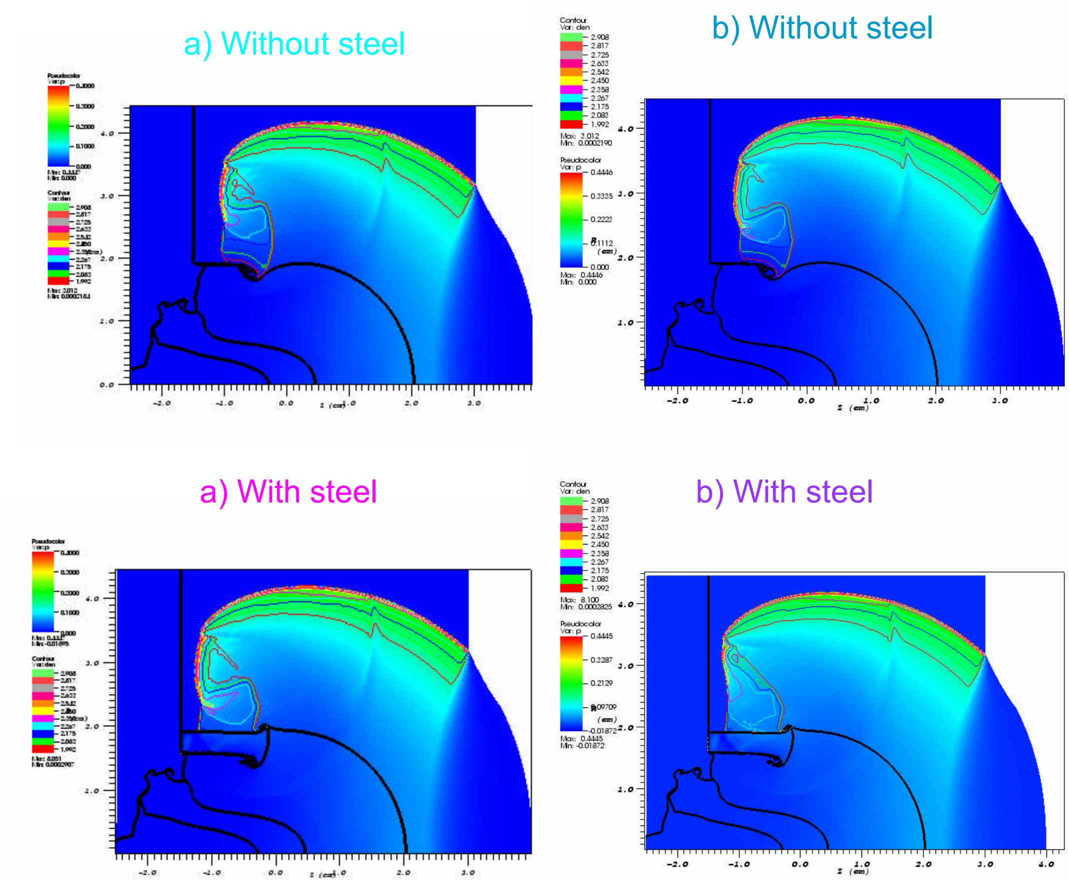
Corner turning modeling LX-17 is sensitive to small changes in the rate pressure profile







Conclusion

- Early calibrations of the Piece Wise Linear reactive flow model have shown that it allows for very accurate agreement with data for a broad range of detonation wave strengths.
- The ability to vary the rate at specific pressures has shown that corner turning involves competition between the strong wave that travels roughly in a straight line and growth at low pressure of a new wave that turns corners sharply.
- The inclusion of a low pressure de-sensitization rate is essential to preserving the dead zone at large times as is observed.